Advancing Materials Modeling to Accelerate Net Shape Fabrication

Current Status and Future Vision

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Incubator Capability Target

A tool for on-demand fabrication of net shape, multifunctional components for aerospace structural applications.

Meeting this target will require significant advances in:

- Printer technology
- CNT fiber reinforced feedstock
- *<u>Methods for optimally designing the components to leverage advances in printer and feedstock</u>*

Why a New Design Method?

Current design methods were created for:

- Metals – subtractive manufacturing
- Composites – sheet/tape prepreg layup manufacturing
- Plastics – molding and extrusion processes

New materials and fabrication process permit:

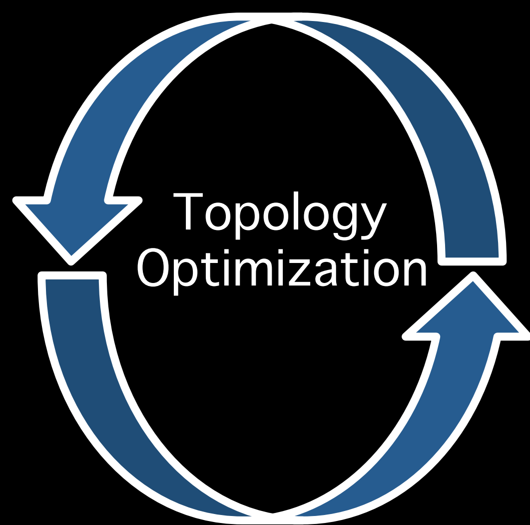
- Optimizing placement/orientation of CNT reinforcement
- Balancing stiffness/strength with mass reduction
- Incorporating electrical and thermal conductivity paths
- Optimizing tool paths for fabrication

Existing design tools cannot do what is required

Topology Optimization

Topology Optimization is an automated technique for optimally designing structures subject to prescribed performance targets and boundary conditions

Structural Design



Material Selection
And Placement

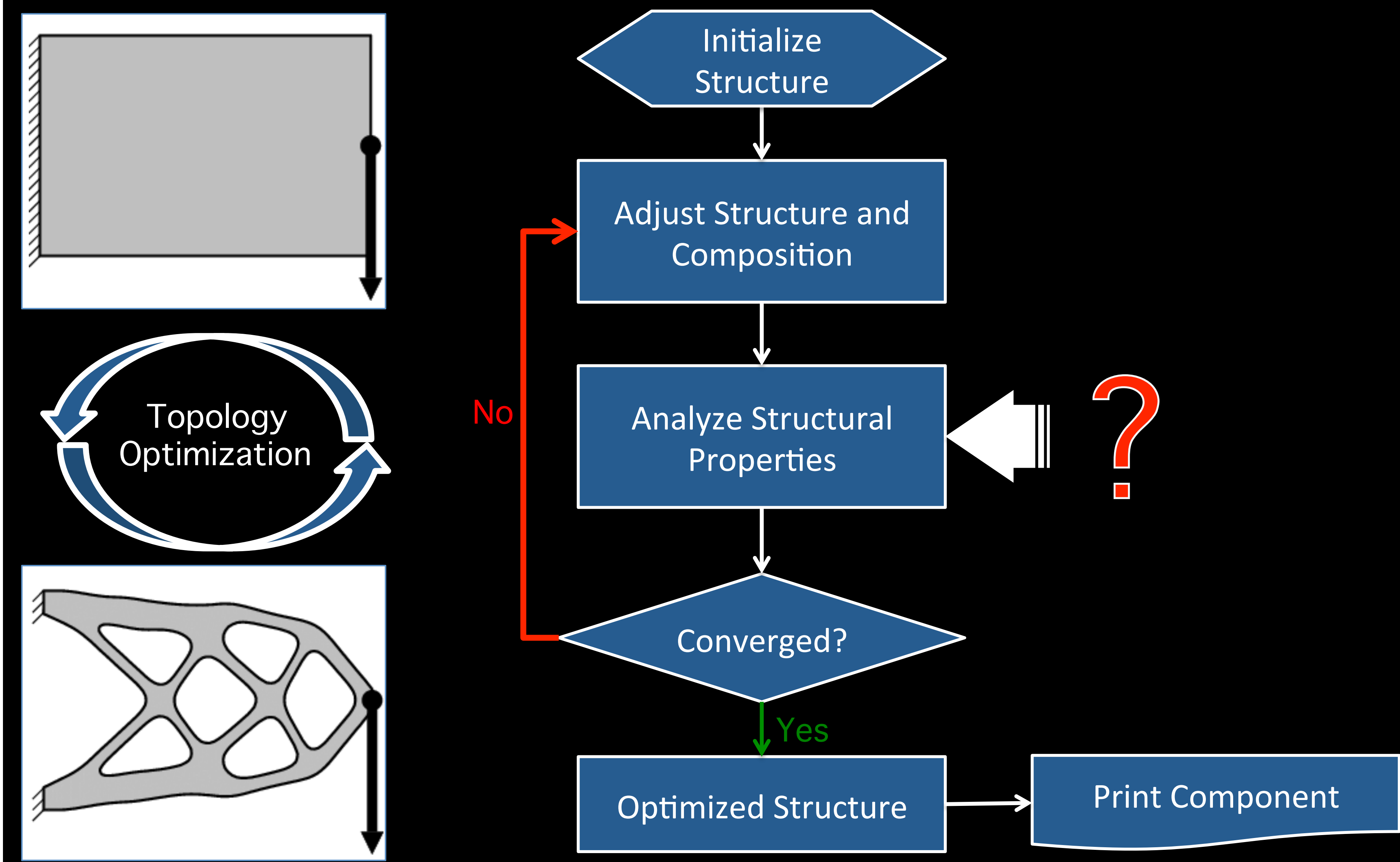
Input

- Loading Requirements
- Mass Constraints
- Dimensional Boundaries
- Material(s) Properties

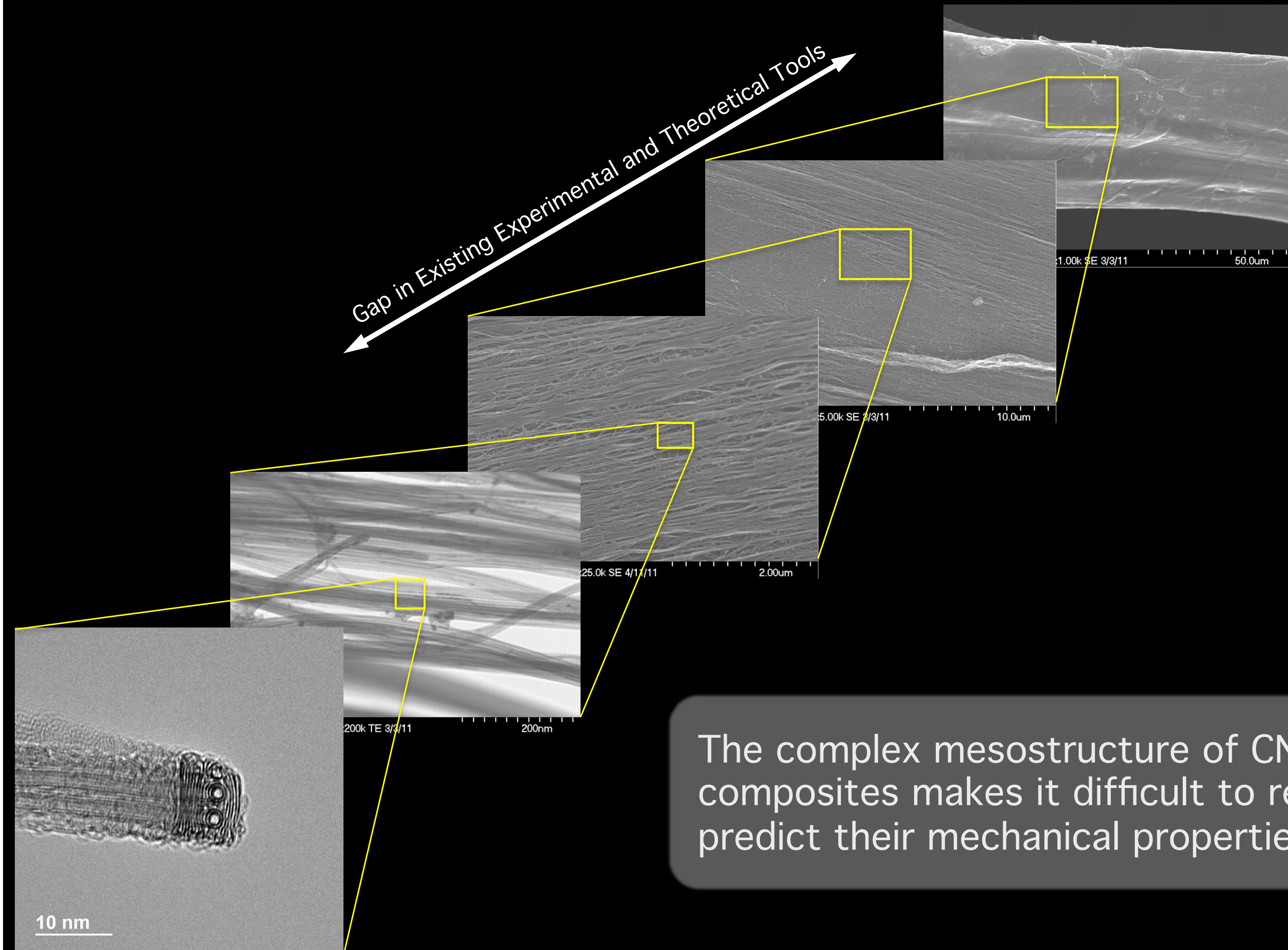
Output

- Component Shape
- Material Distribution
- Loading Capacity
- Response Properties

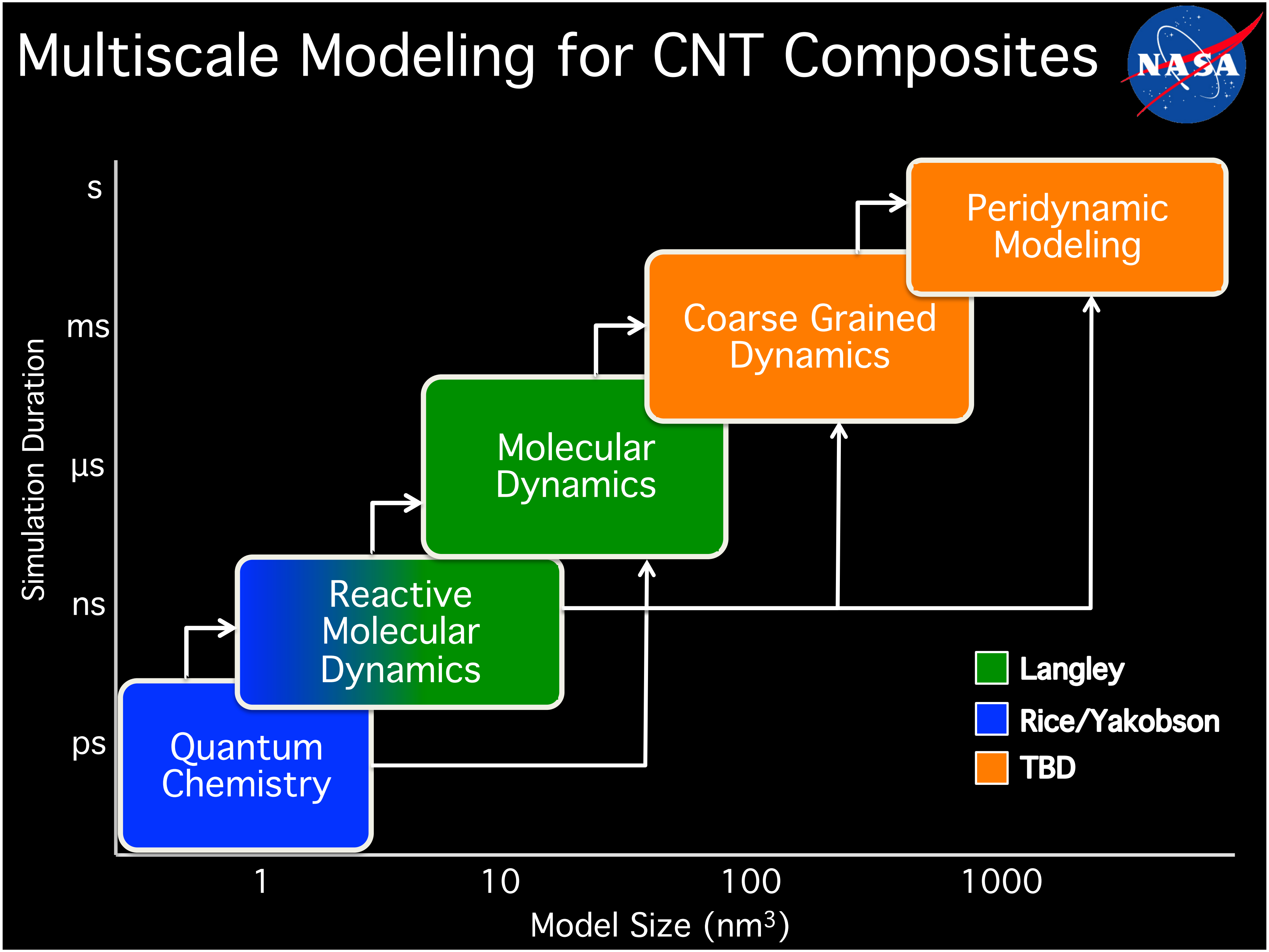
Topology Optimization Flow Chart



Multiscale Structure of CNT Fibers



The complex mesostructure of CNT composites makes it difficult to reliably predict their mechanical properties



Multiscale Modeling for CNT Composites
NASA
Simulation Duration
s
ms
µs
ns
ps
Quantum Chemistry
Reactive Molecular Dynamics
Molecular Dynamics
Coarse Grained Dynamics
Peridynamic Modeling
Langley
Rice/Yakobson
TBD
1
10
100
1000
Model Size (nm³)

What is Peridynamic Modeling?

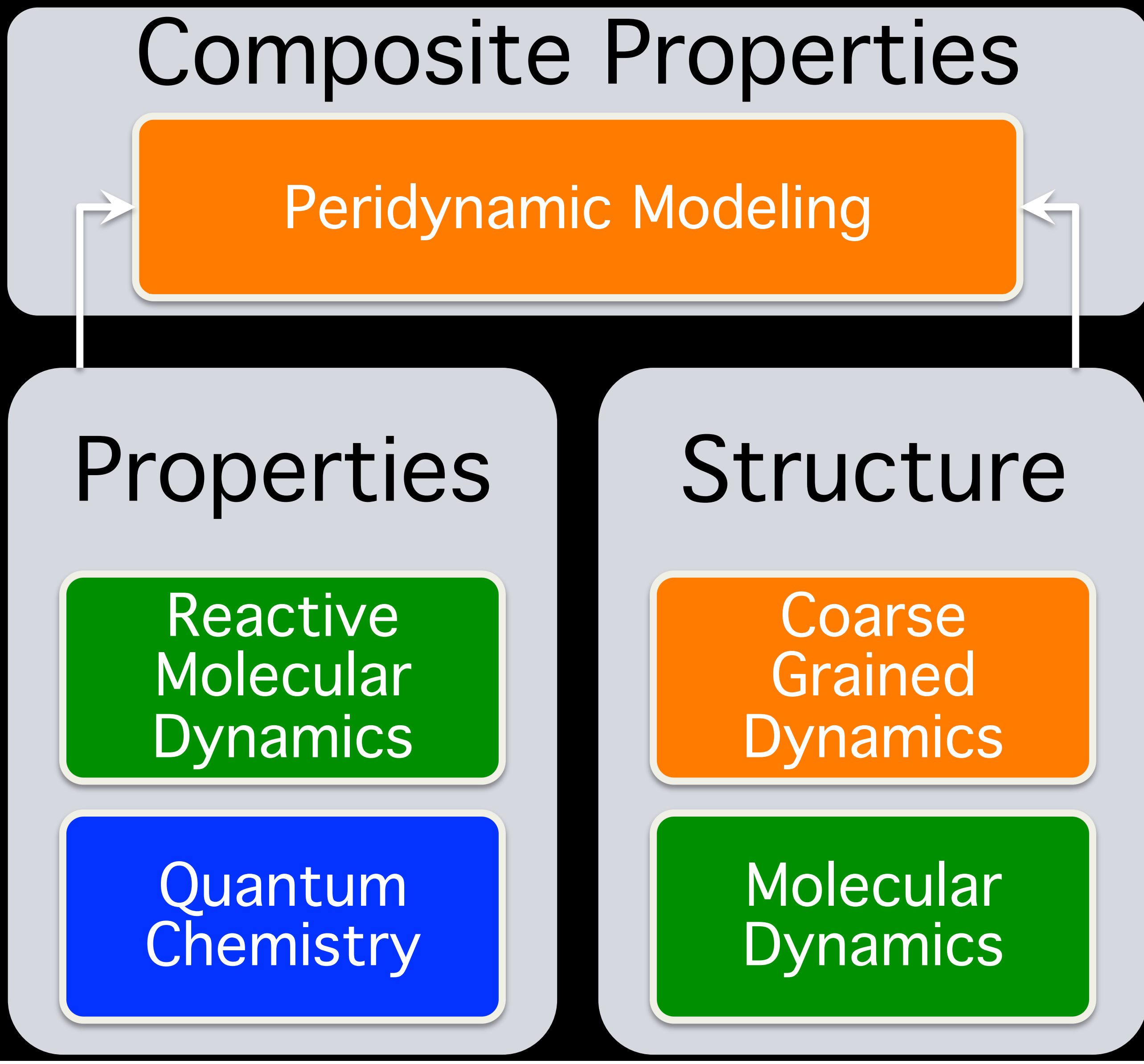
A recent method with exciting capabilities:

- Introduced in 2000, still in active development
- Represents continuum materials with material points
- Nonlocal theory that bridges from finite element to molecular dynamics via an adjustable internal length parameter

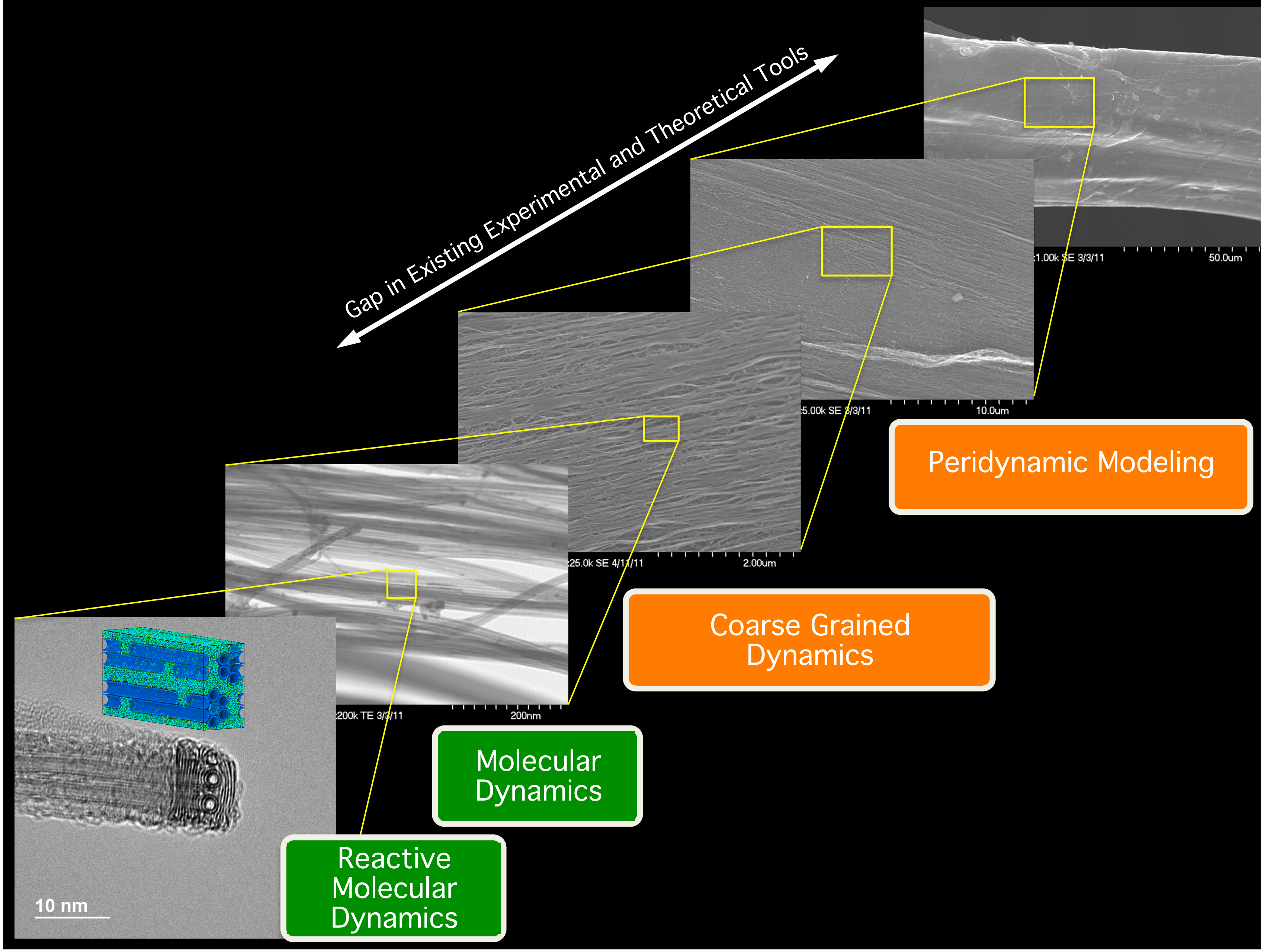
Particularly for CNT fiber composite materials:

- Damage initiation and propagation at multiple sites
- Arbitrary fracture paths without special crack growth criteria
- Permits arbitrary numbers and shapes of inclusions and voids
- Material properties depend on detailed micro/mesostructure

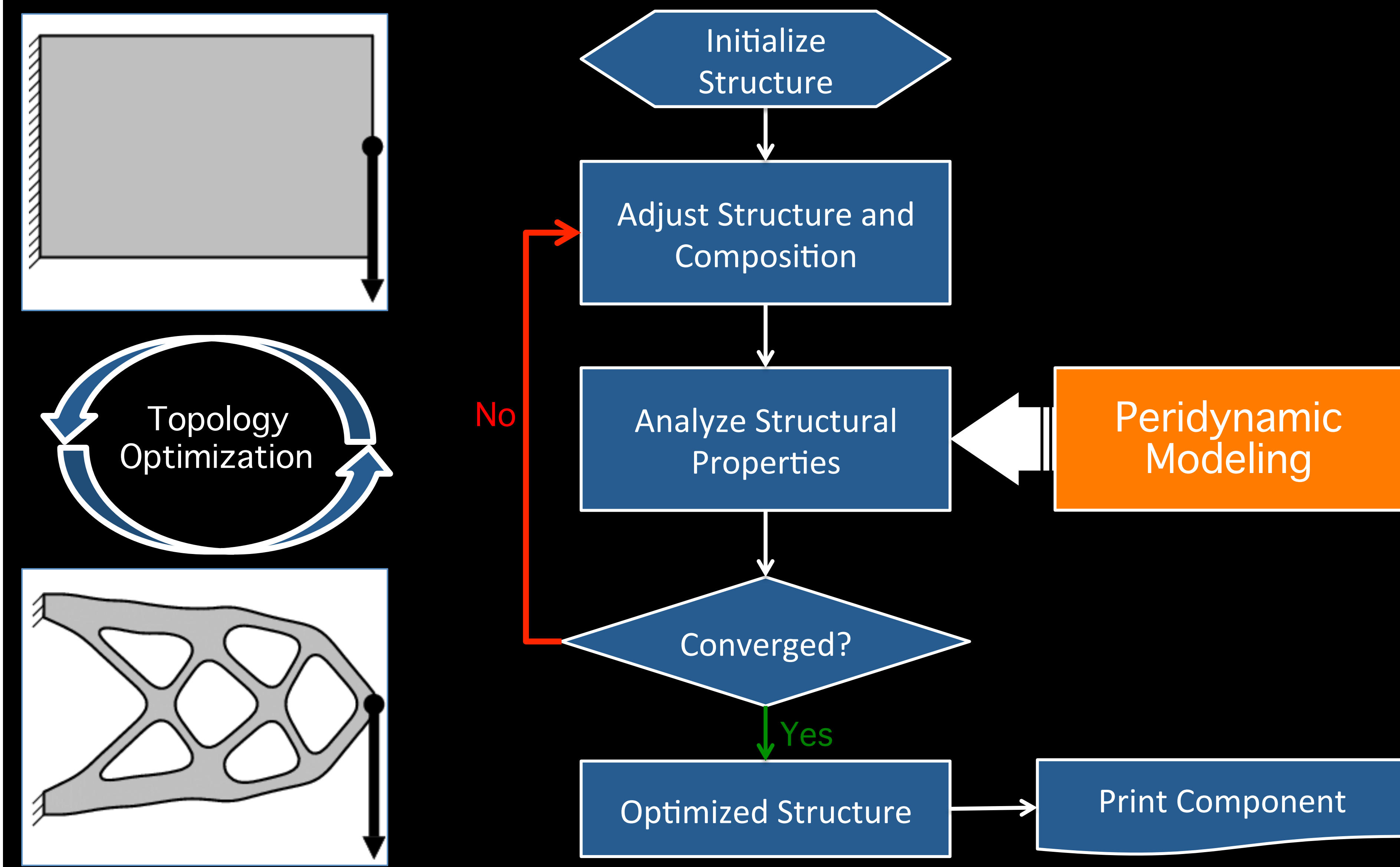
Multiscale Modeling for CNT Composites



Multiscale Structure of CNT Fibers



Topology Optimization Flow Chart



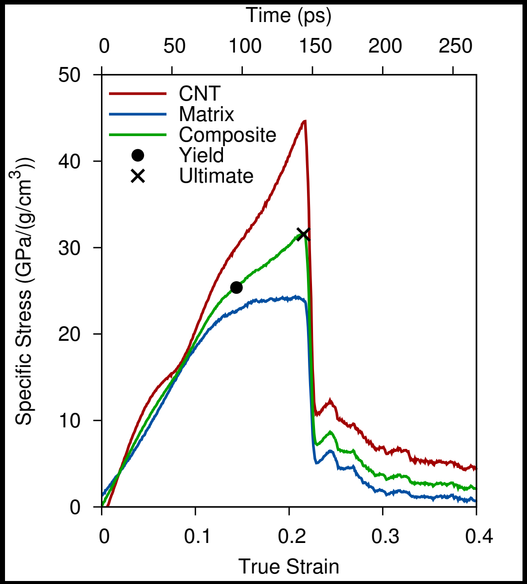
Recent LaRC Modeling Work

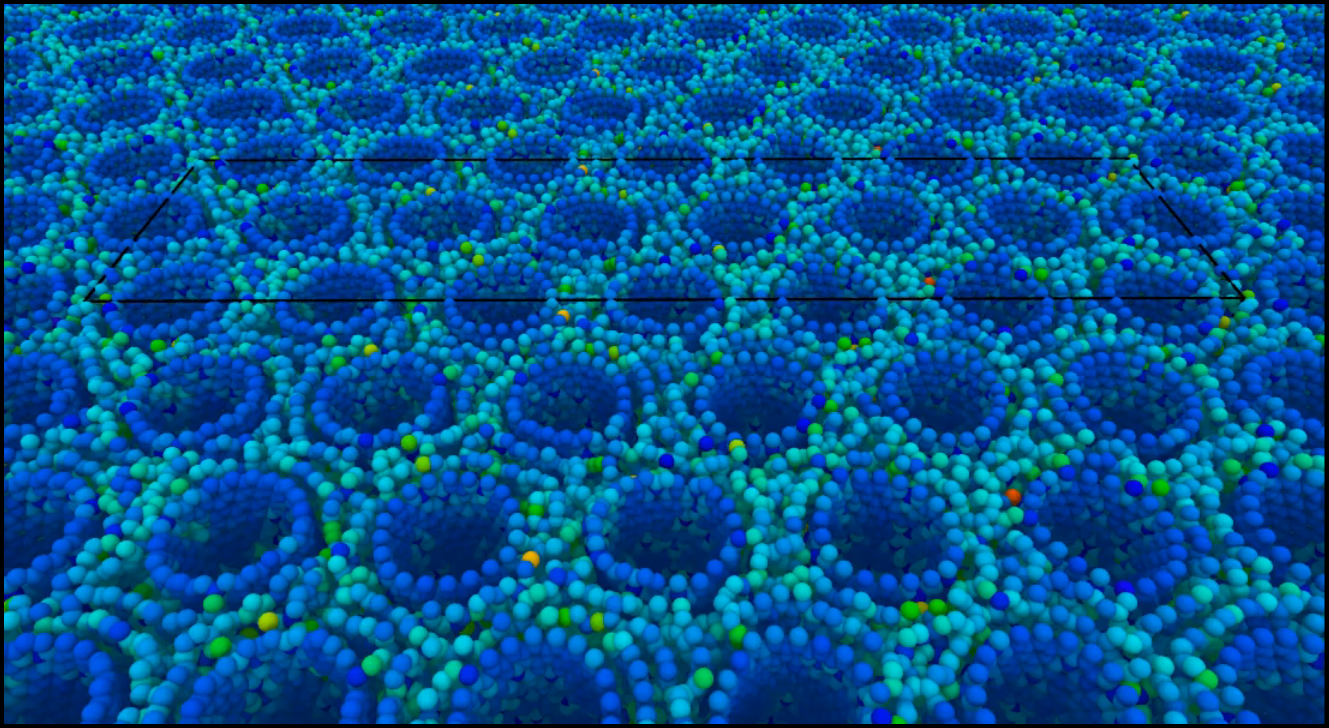
Reactive Molecular Dynamics Simulations of CNT/Amorphous Carbon Composites

Ben Jensen, Kris Wise (LaRC)
Greg Odegard (MTU)

Fracture of CNT Composites

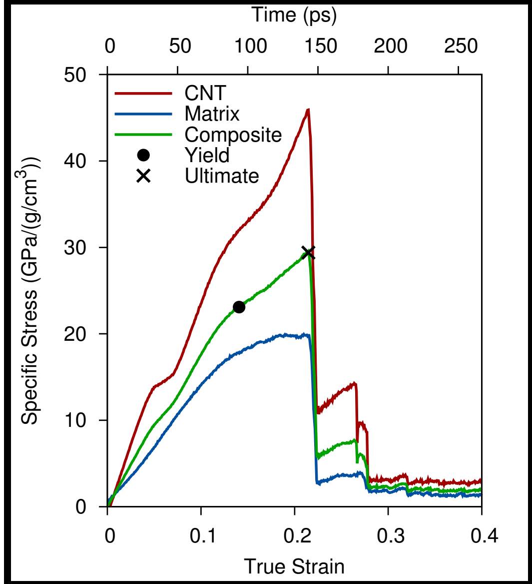
ReaxFF Simulation of a SWNT Array/Amorphous Carbon Composite

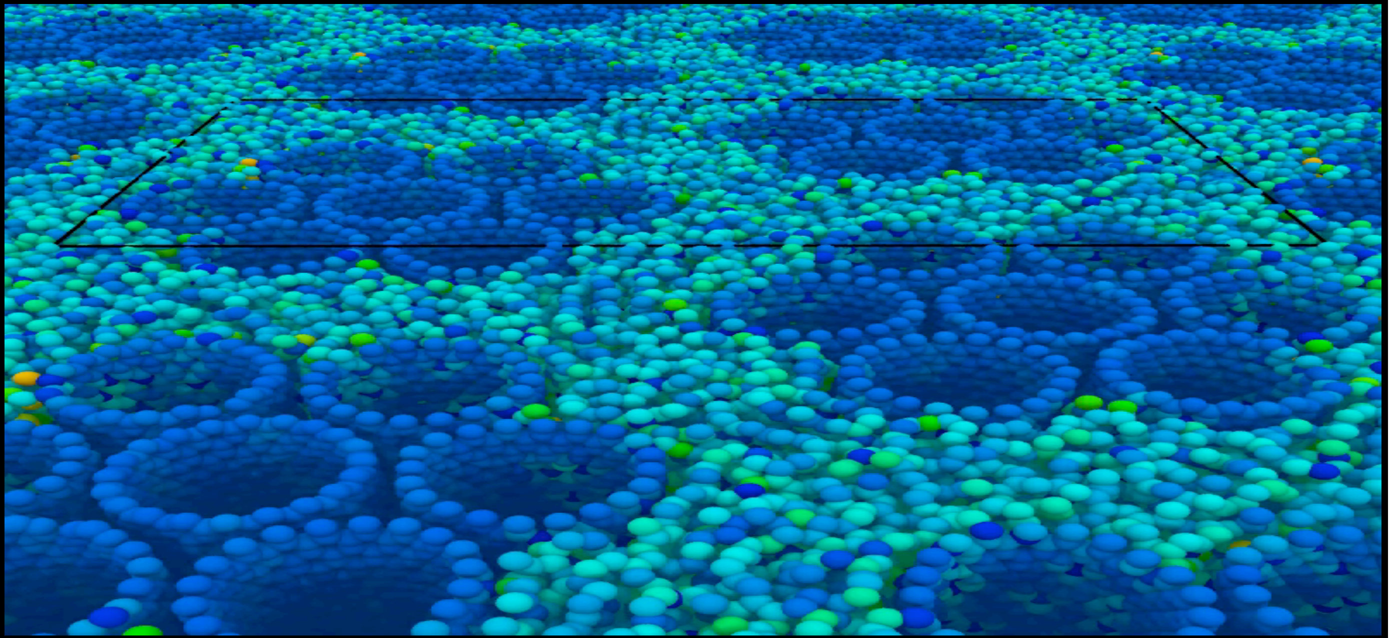




Fracture of CNT Composites

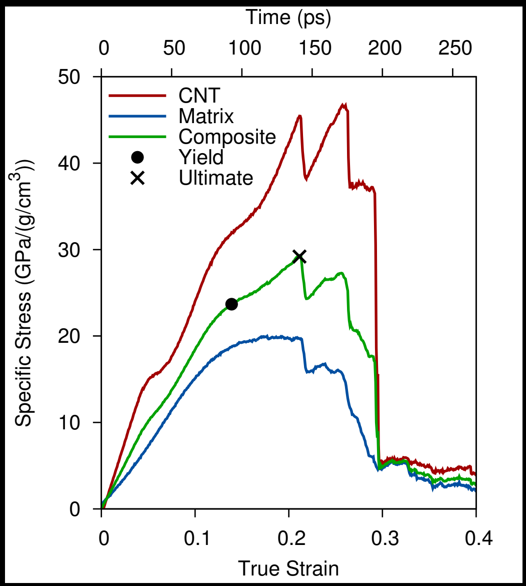
ReaxFF Simulation of a SWNT Bundle/Amorphous Carbon Composite

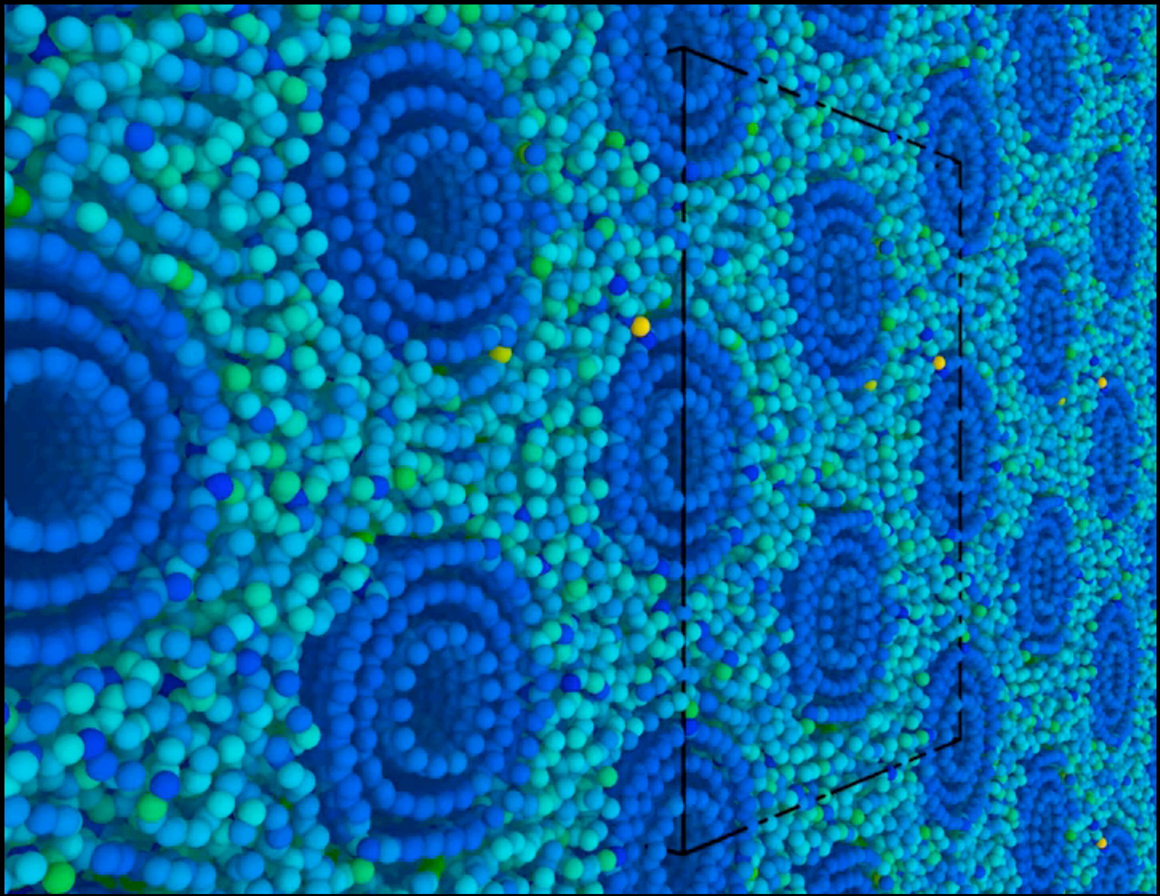




Fracture of CNT Composites

ReaxFF Simulation of a MWNT Array/Amorphous Carbon Composite

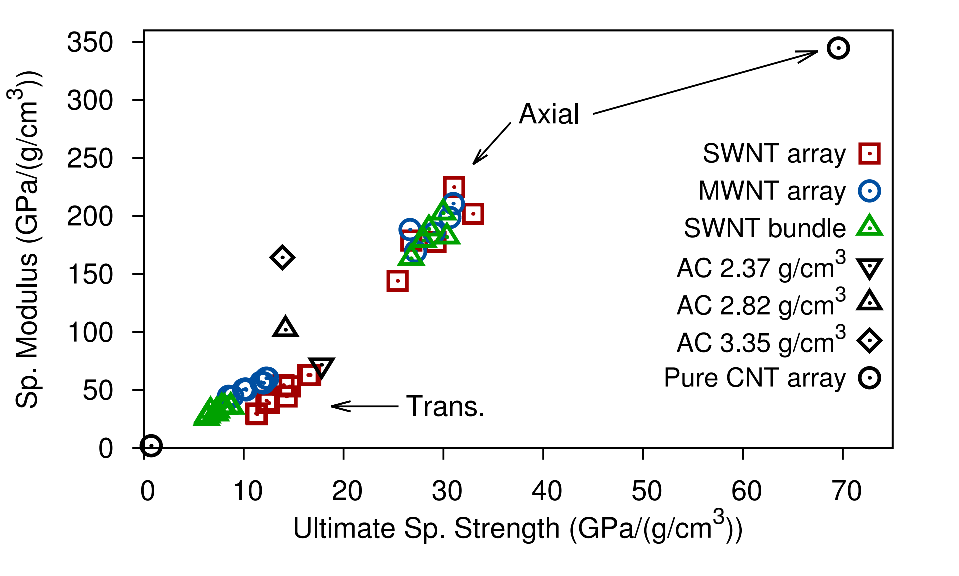




Summary of Fracture Results

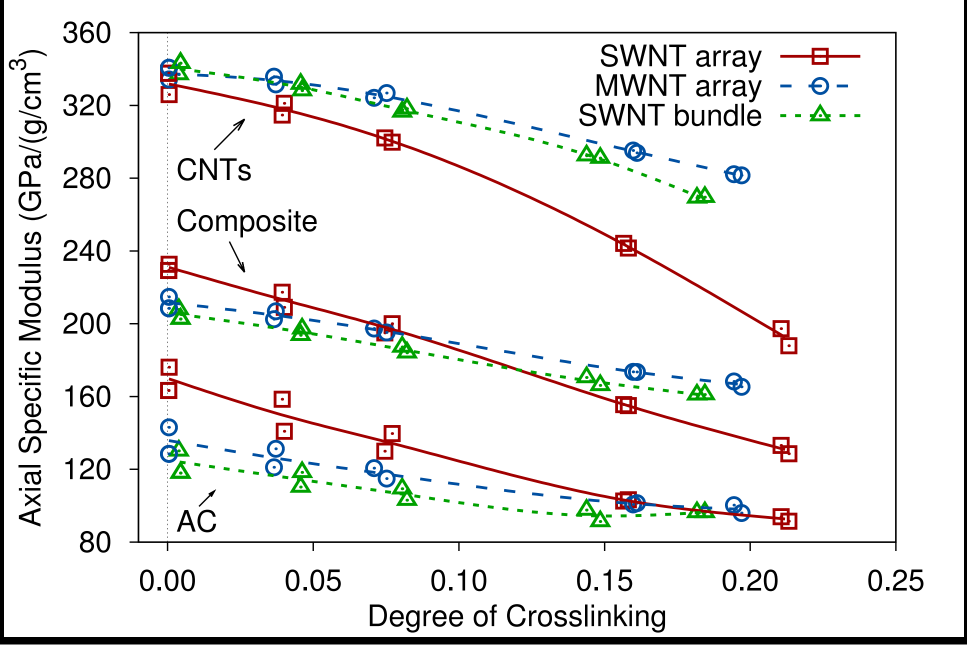
Trends in Mechanical Properties

- Axial specific moduli ≈200 GPa, axial specific strength ≈ 30 GPa
- Transverse specific moduli ≈ 50 GPa, transverse specific strengths ≈ 10 GPa
- These results place an upper bound on expected experimental results



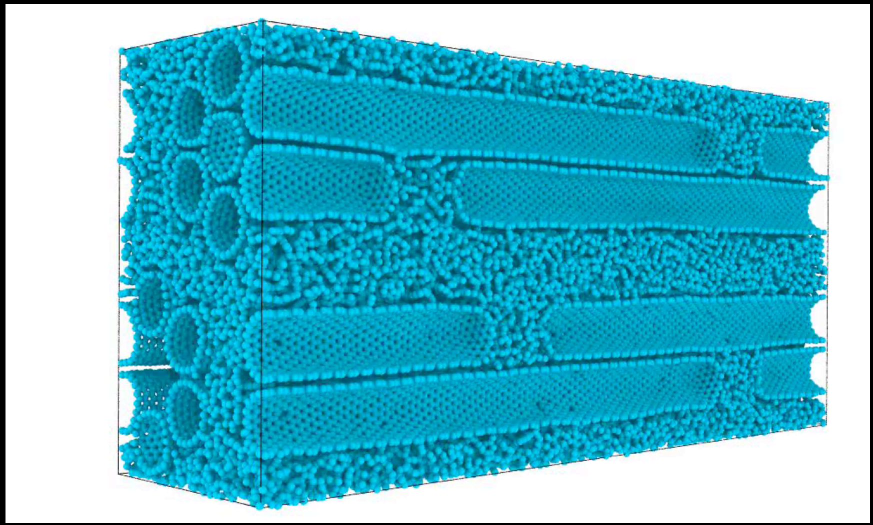
Effect of Crosslinking to the Matrix

- SWNT Array most sensitive to crosslinking, which is reduced by bundling
- Smallest reduction in specific modulus found for MWNT array
- Loss in axial properties compensated for by increase in transverse directions

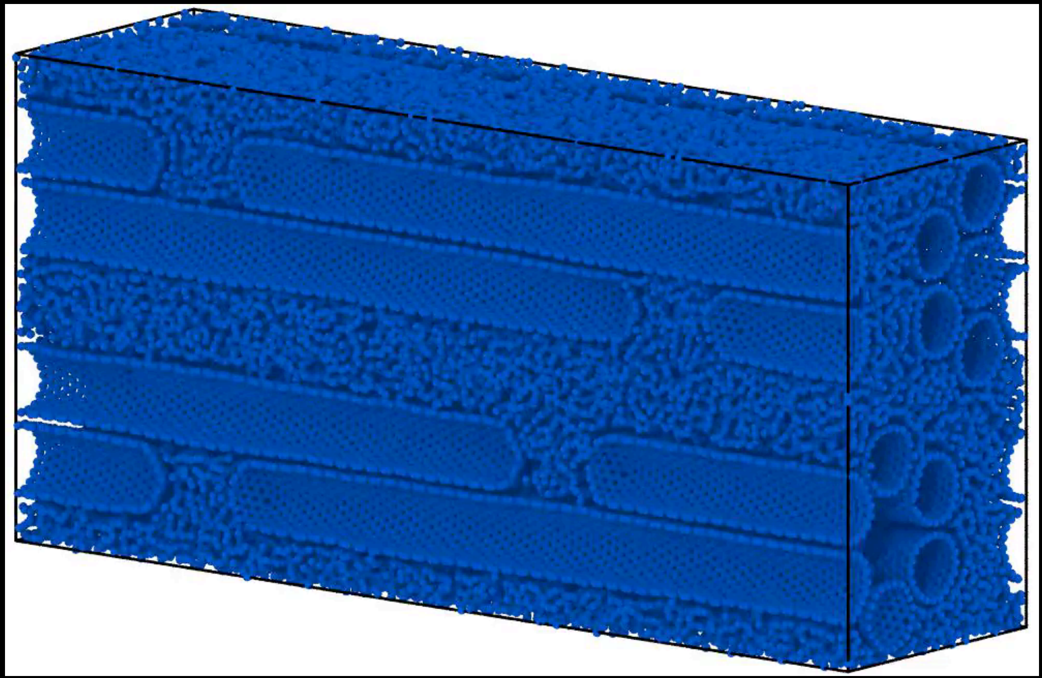


Discontinuous SWNT Bundles

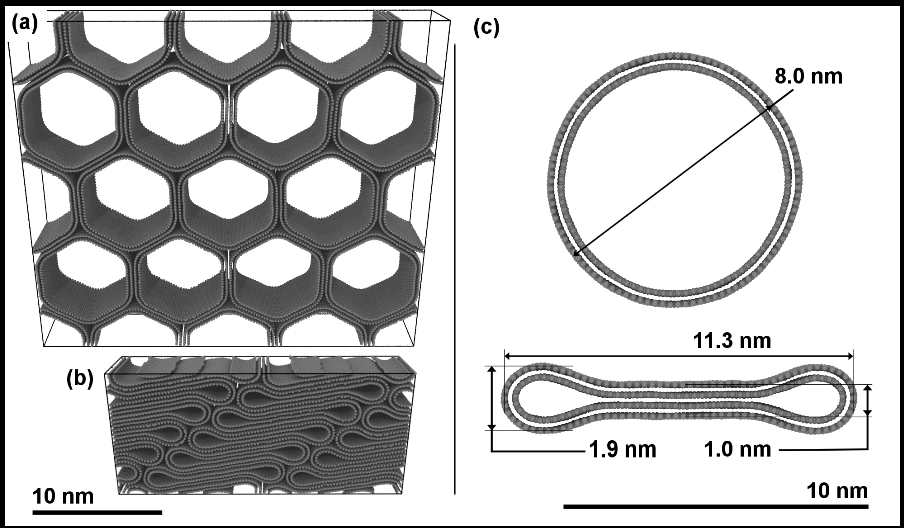
Tension

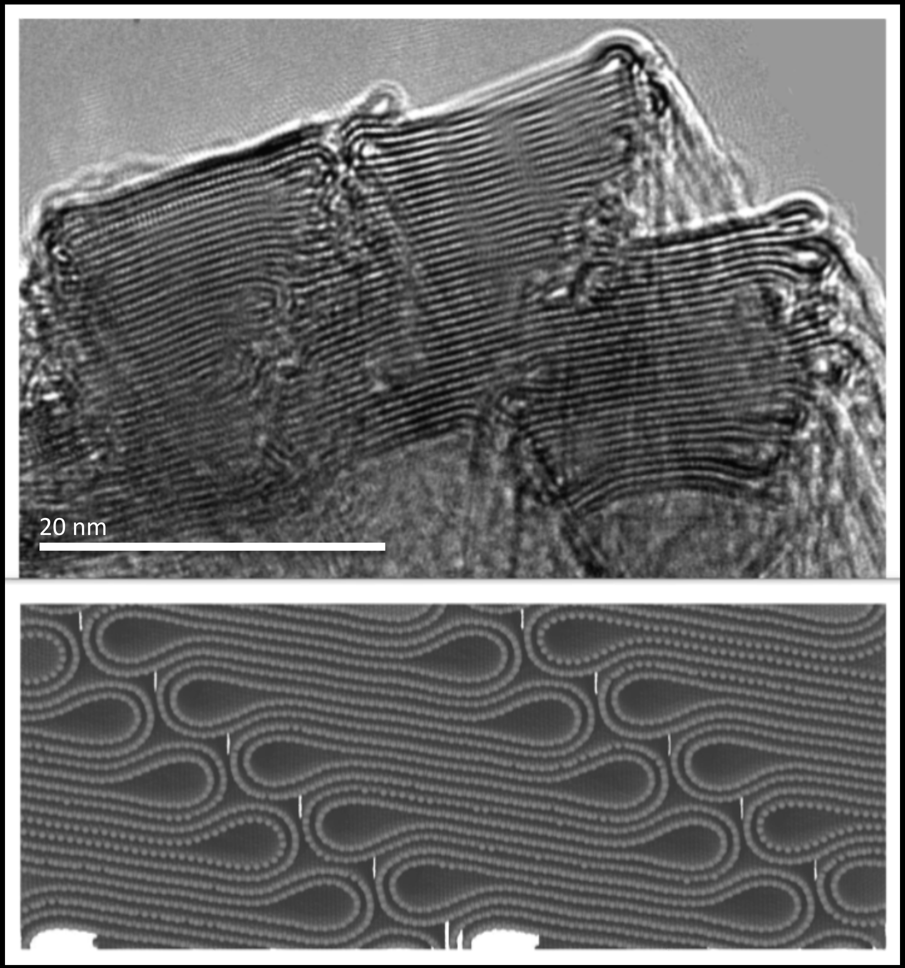


Compression



Collapse of Large Diameter CNTs





Acknowledgements

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- Erdogan Madenci, U Arizona